

Dantrolene
7261-97-4 | DTXSID7022881

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.00e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 3.83e-01

Confidence level: 5.97e-01

Nearest Neighbors from the Training Set

Image not found

Thalidomide

Measured: 2.11e-03

Predicted: 5.89e-03

Image not found

Benomyl

Measured: 1.31e-05

Predicted: 3.43e-03